

**CINTRA-CDPT Joint Seminar Presented by:**

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**Title: Controlling Leakage Currents in Molecular Electronic Devices**

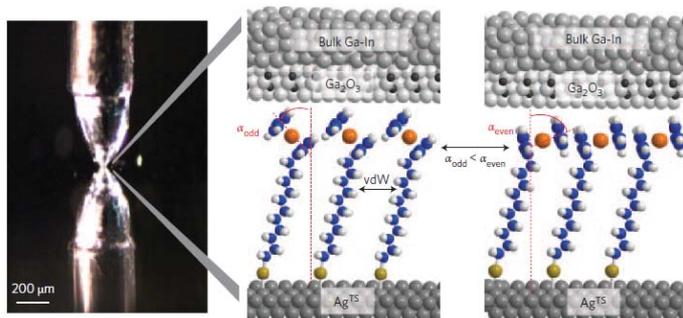
Date: Friday, 15<sup>th</sup> November 2013

Time: 15:00-16:30

Venue: SPMS MAS Executive Classroom 1 (SPMS-MAS-03-06)

**Abstract**

One of the major goals of molecular electronics is to relate the performance and electronic function of these devices to the chemical structure and intermolecular interactions of the organic molecules inside them. Molecular electronic devices are complex physical-organic systems that consist of at least two electrodes, the organic component, and two (different) organic/inorganic interfaces. Singling out the contribution of each of these components to the device performance is not straightforward. So far, strong  $\pi$ - $\pi$  interactions have mainly been considered for the rational design and optimization of the performances of organic electronic devices, whereas weaker intermolecular interactions have been largely ignored.<sup>1</sup> Here we experimentally show that subtle changes in the intermolecular van der Waals interactions in the active component of a molecular diode dramatically impact the performance of the device (See Figure).<sup>2</sup> In particular, we observe an odd-even effect as the number of  $-CH_2-$  units are varied in a ferrocene-alkanethiolate SAM: as a result of a more favourable van der Waals interaction, junctions made from an odd number of alkyl units have a lower packing energy by approximately 0.4-0.6 kcal mol<sup>-1</sup> and rectify currents 10 times more efficiently, give 10% higher yield of working devices and can be made 2-3 times more reproducibly than junctions made from an even number of alkyl units. Besides subtle changes in the packing energy, we also showed that preparation of the bottom-electrode (especially grain boundaries), the type of the anchoring group, and the purity of the SAM precursor are crucial. Once the supramolecular structure can be controlled, the electronic structure can also be controlled which we used to turn around a diode at the molecular level.



The Figure shows a junction with liquid metal alloy of Ga and In top-contacts, SAMs of  $S(CH_2)_nFc$  ( $n = 10$  or  $11$ ; Fc = ferrocene) on silver bottom-contacts. A small variation of the tilt angle of the Fc units resulted in a remarkable odd-even effect in the performance of the junctions

**References**

- [1] Henson, Z. B., Müllen, K., Bazan, G. C. *Nature Chem.* 4, 699-704 (2012).  
 [2] Nerngchamnong, N., Yuan, Li., Qi, D.C., Li, J., Thompson, D., Nijhuis, C. A. *Nature Nano.* DOI: 10.1038/NNANO.2012.238

**About Speaker**



Christian A. Nijhuis received his Masters degree in Chemistry from the University of Groningen in 2002, and Ph.D. degree from University of Twente in 2006 (Cum Laude; top 5%). Under the direction of Professor David N. Reinhoudt, his doctoral thesis included studies on the surface chemistry of supramolecular assemblies and their use in bottom-up nano-fabrication. He received the Simon Stevin Research award from the Netherlands Organization for Scientific Research (NWO) in 2006 to conduct overseas research. In the group of Professor George M. Whitesides, as a postdoctoral research fellow, he developed a platform for measurements of charge transport across layers that are one molecule thick. In

2010, he received the NRF research fellowship and he joined the Department of Chemistry at the National University of Singapore as an Assistant Professor. He currently uses bottom-up nanofabrication techniques to construct self-assembled nano-electronic devices to open up and to solve key problems in physics